

10552362a

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:20:17 ON 02 APR 2007

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:20:27 ON 02 APR 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2007 HIGHEST RN 928822-97-3

DICTIONARY FILE UPDATES: 1 APR 2007 HIGHEST RN 928822-97-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

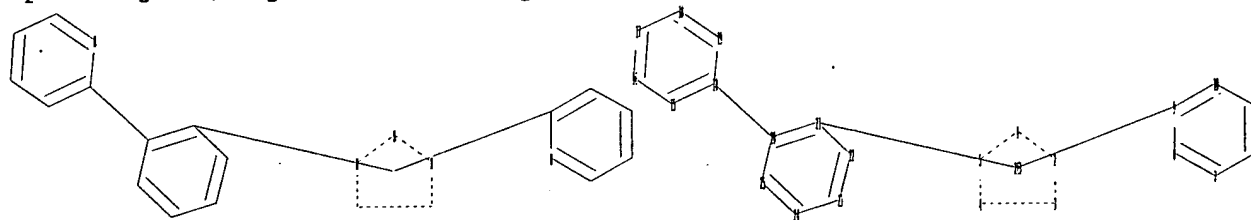
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res1.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

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chain bonds :

14-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-21 20-25 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-21
20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 :

Match level :

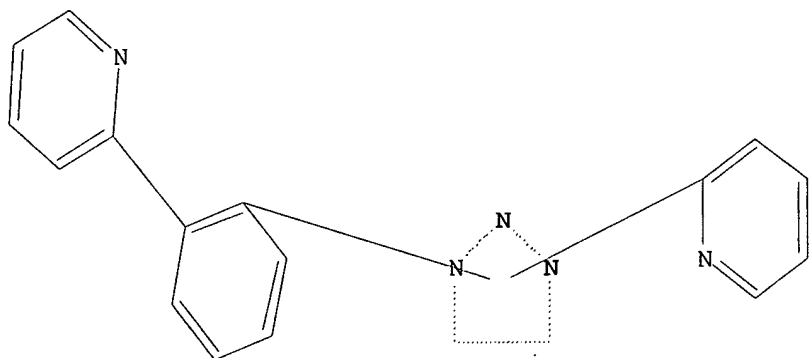
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:20:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1535 TO ITERATE

100.0% PROCESSED 1535 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

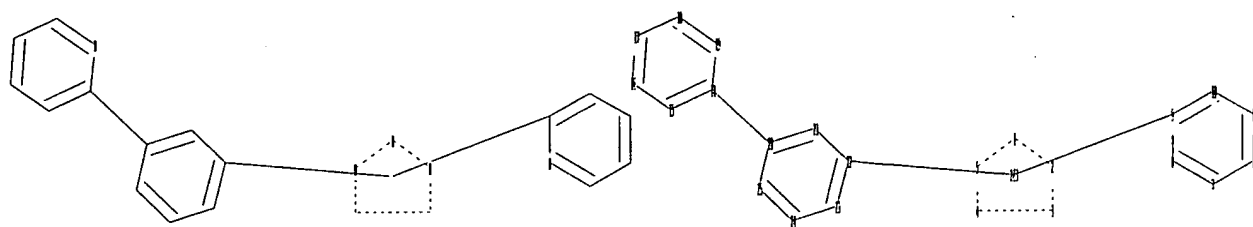
L2 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res2.str

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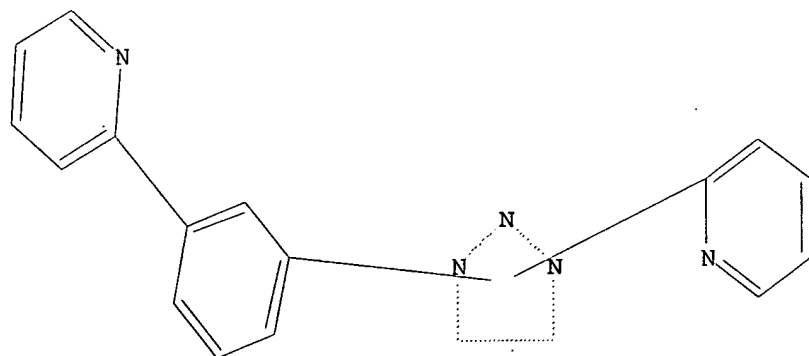


ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
14-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-21
20-25 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



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Structure attributes must be viewed using STN Express query preparation.

=> s l3 full

FULL SEARCH INITIATED 14:21:41 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

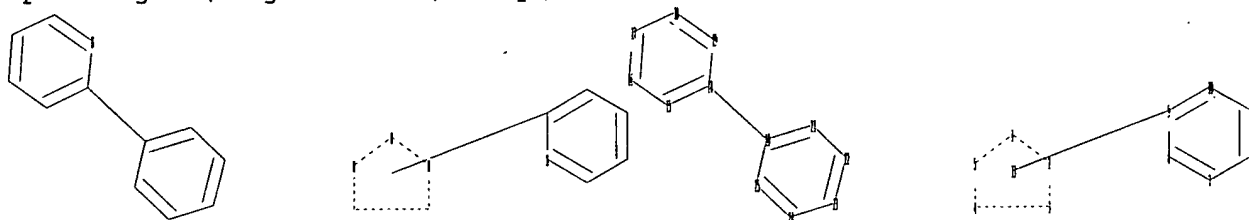
2 ANSWERS

SEARCH TIME: 00.00.01

L4 2 SEA SSS FUL L3

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res3.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

14-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16

16-17 17-18 18-19 20-21 20-25 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-21

20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom

L5 STRUCTURE UPLOADED

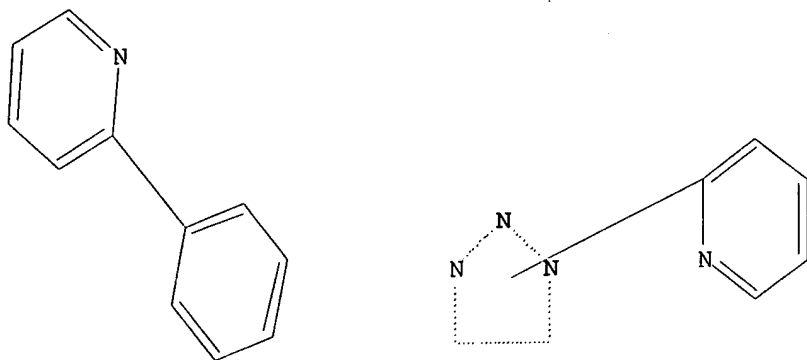
=> d

L5 HAS NO ANSWERS

L5 STR

Karen Cheng

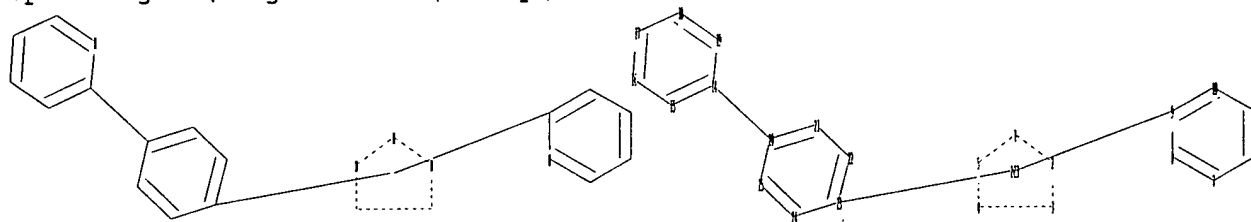
10552362a



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res4.str



ring nodes :
1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
14-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5
exact bonds :
14-20
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-21
20-25 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

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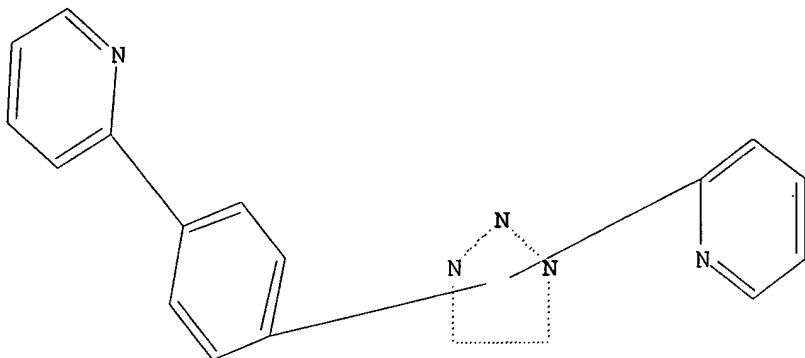
10552362a

L6 STRUCTURE UPLOADED

=> d

L6 HAS NO ANSWERS

L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l6 full

FULL SEARCH INITIATED 14:23:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

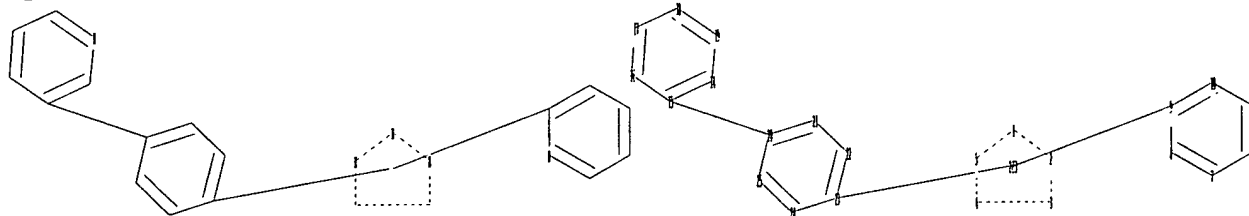
8 ANSWERS

SEARCH TIME: 00.00.01

L7 8 SEA SSS FUL L6

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res5.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

15-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-20

normalized bonds :

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7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
20-21 21-22 22-23 23-24 24-25
isolated ring systems :
containing 1 : 7 : 14 : 20 :

Match level :

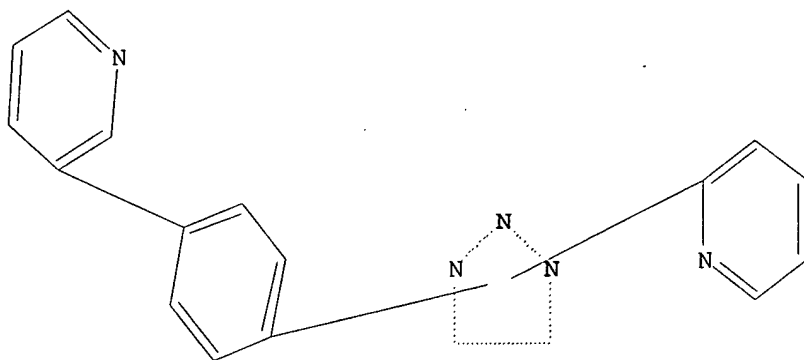
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L8 STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l8 full

FULL SEARCH INITIATED 14:24:13 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

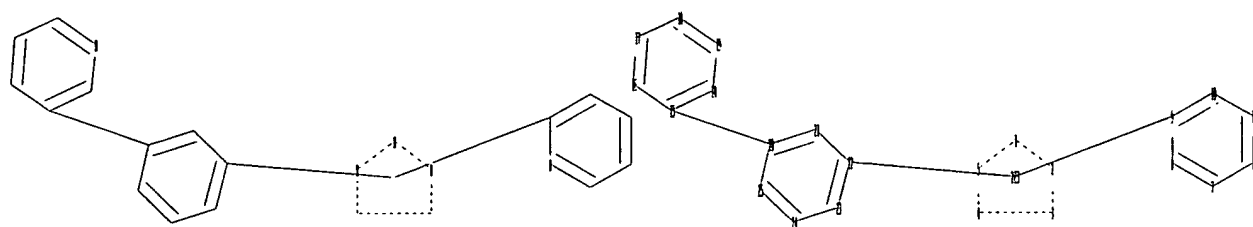
L9 0 SEA SSS FUL L8

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res6.str

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ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

15-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

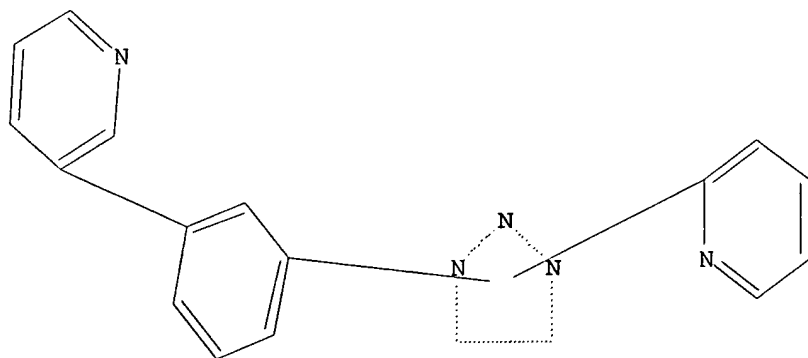
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

L10 STR



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Structure attributes must be viewed using STN Express query preparation.

=> s l10 full

FULL SEARCH INITIATED 14:25:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

2 ANSWERS

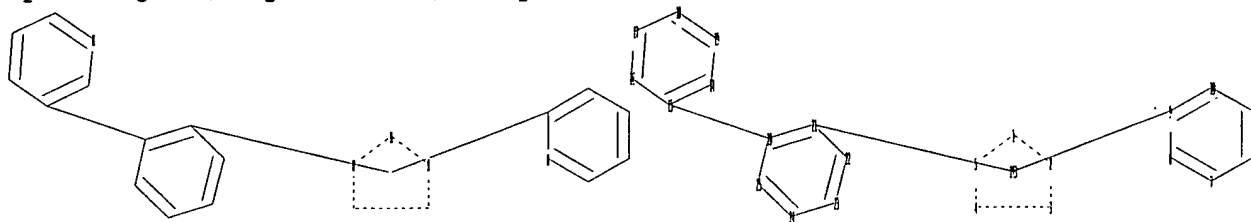
SEARCH TIME: 00.00.01

L11

2 SEA SSS FUL L10

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res7.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

15-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L12 STRUCTURE UPLOADED

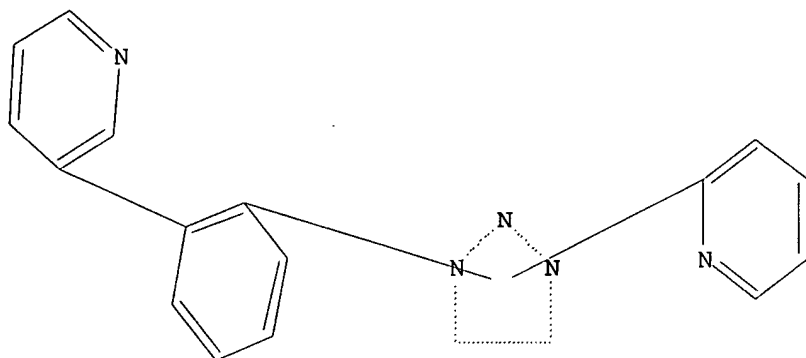
=> d

L12 HAS NO ANSWERS

L12 STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l12 full

FULL SEARCH INITIATED 14:25:47 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

0 ANSWERS

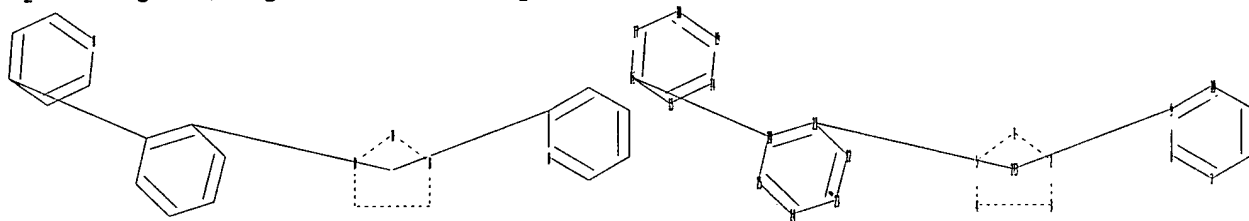
SEARCH TIME: 00.00.01

L13

0 SEA SSS FUL L12

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res8.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

16-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16

16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

16-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25

20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

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Match level :

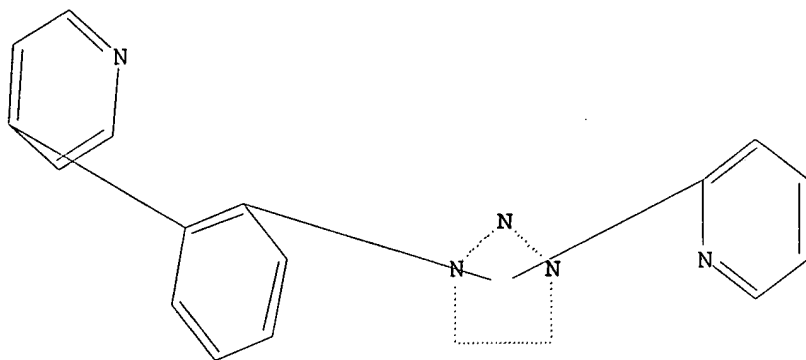
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L14 STRUCTURE UPLOADED

=> d

L14 HAS NO ANSWERS

L14 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l14 full

FULL SEARCH INITIATED 14:26:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

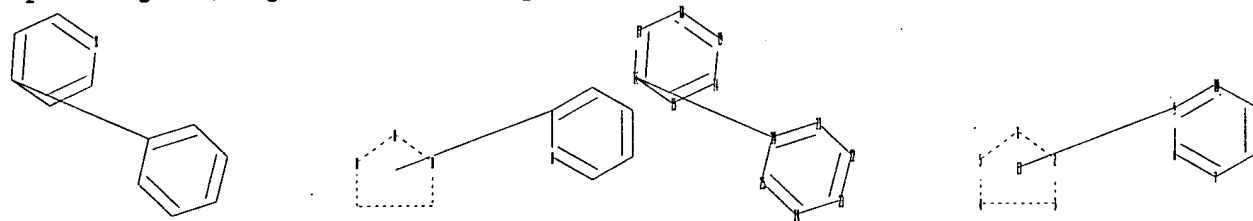
0 ANSWERS

SEARCH TIME: 00.00.01

L15 0 SEA SSS FUL L14

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res9.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

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16-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

16-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

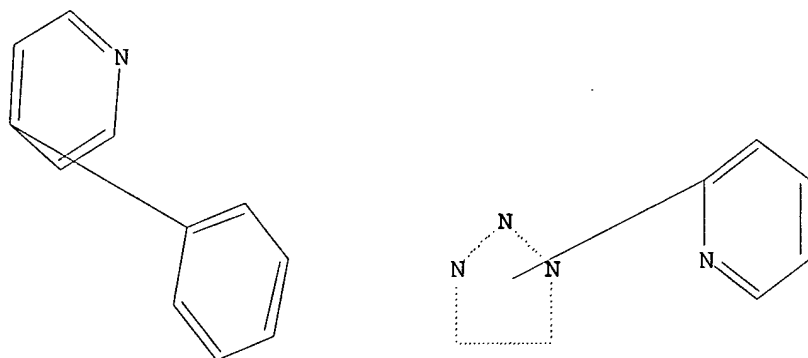
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom

L16 STRUCTURE UPLOADED

=> d

L16 HAS NO ANSWERS

L16 STR



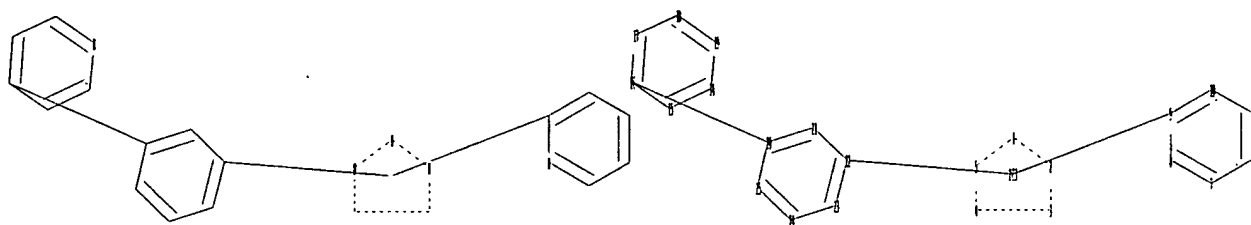
Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res10.str

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10552362a



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

16-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16
16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

16-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25
20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

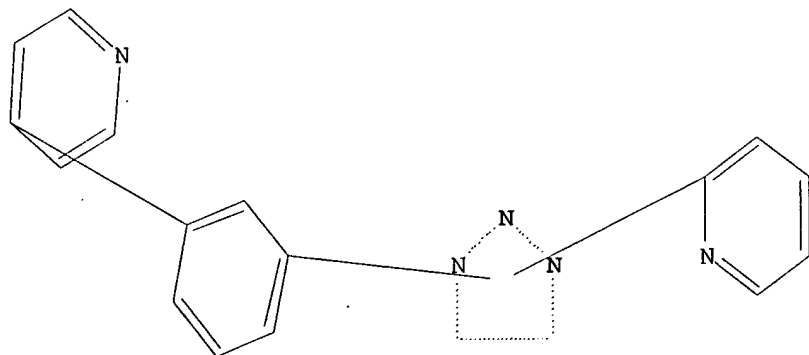
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L17 STRUCTURE UPLOADED

=> d

L17 HAS NO ANSWERS

L17 STR



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10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l17 full

FULL SEARCH INITIATED 14:28:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

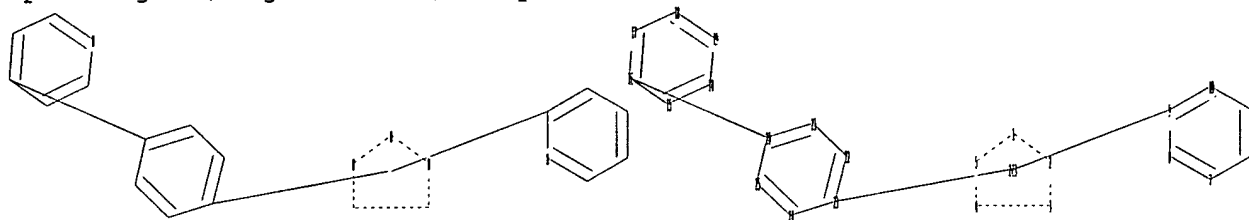
SEARCH TIME: 00.00.01

L18

0 SEA SSS FUL L17

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res11.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25

chain bonds :

16-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16

16-17 17-18 18-19 20-25 20-21 21-22 22-23 23-24 24-25

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

16-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 14-19 14-15 15-16 16-17 17-18 18-19 20-25

20-21 21-22 22-23 23-24 24-25

isolated ring systems :

containing 1 : 7 : 14 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L19 STRUCTURE UPLOADED

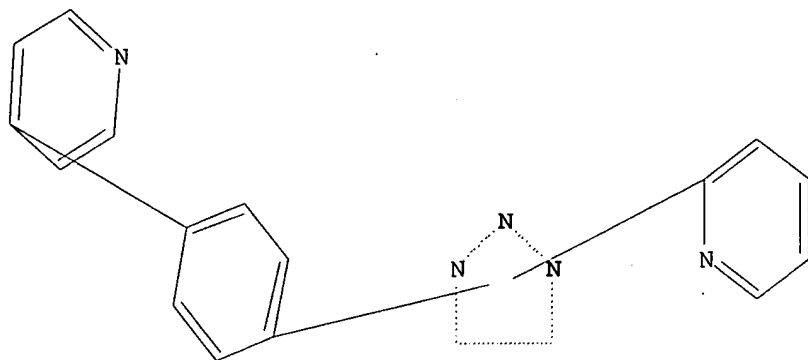
=> d

L19 HAS NO ANSWERS

L19 STR

Karen Cheng

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Structure attributes must be viewed using STN Express query preparation.

=> s 119 full

FULL SEARCH INITIATED 14:29:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

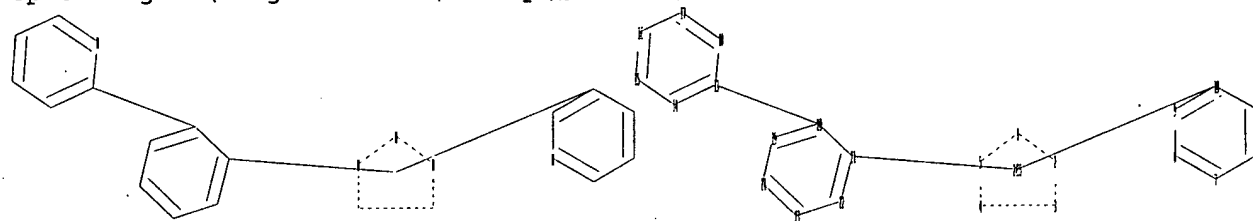
SEARCH TIME: 00.00.01

L20

0 SEA SSS FUL L19

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res12.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

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10552362a

Match level :

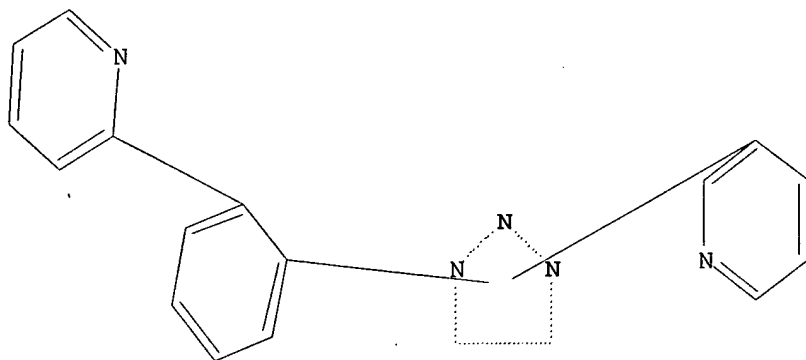
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L21 STRUCTURE UPLOADED

=> d

L21 HAS NO ANSWERS

L21 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l21 full

FULL SEARCH INITIATED 14:31:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

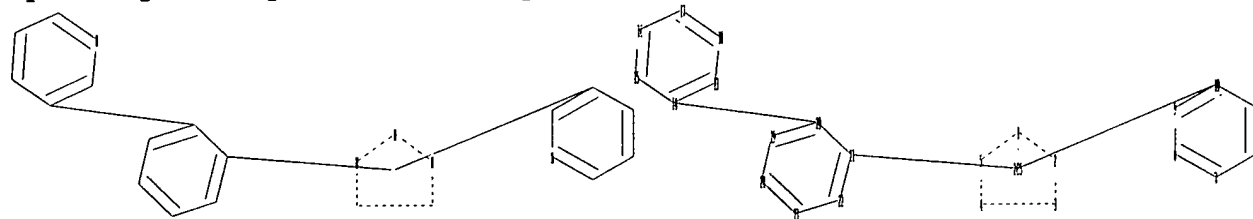
0 ANSWERS

SEARCH TIME: 00.00.01

L22 0 SEA SSS FUL L21

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res13.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

Karen Cheng

10552362a

14-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

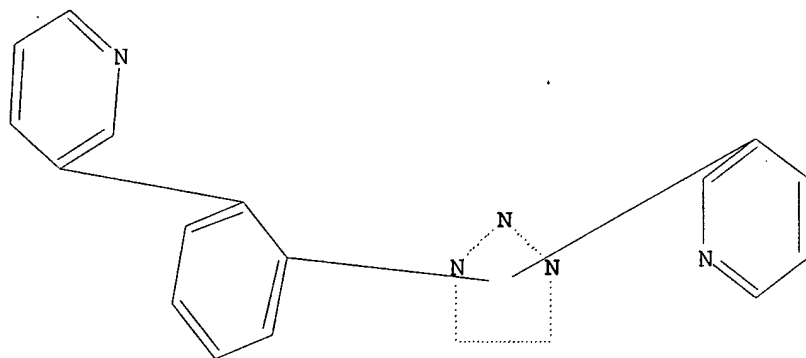
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L23 STRUCTURE UPLOADED

=> d

L23 HAS NO ANSWERS

L23 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l23 full

FULL SEARCH INITIATED 14:31:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

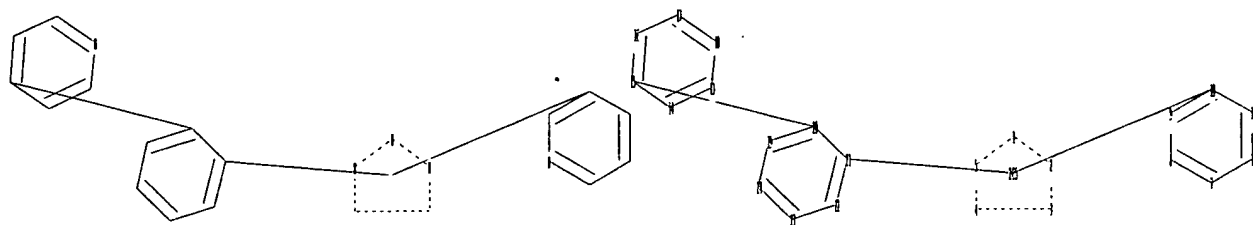
L24 0 SEA SSS FUL L23

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res14.str

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10552362a



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

15-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

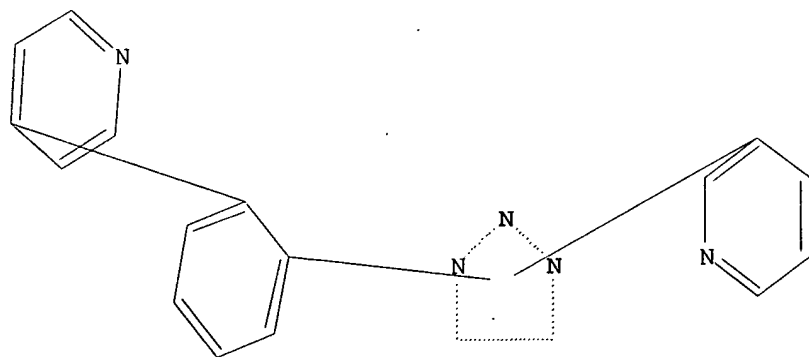
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L25 STRUCTURE UPLOADED

=> d

L25 HAS NO ANSWERS

L25 STR



Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l25 full

FULL SEARCH INITIATED 14:32:25 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

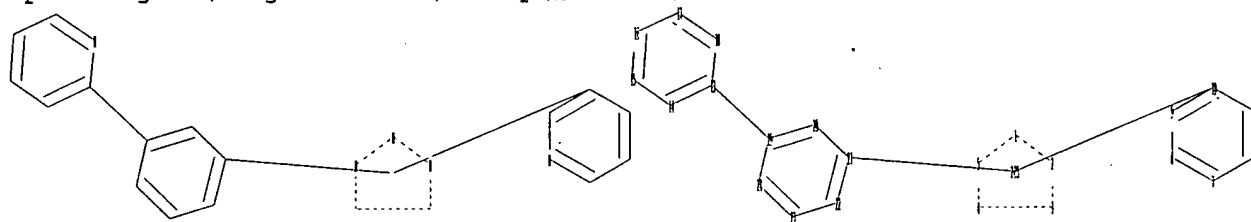
SEARCH TIME: 00.00.01

L26

0 SEA SSS FUL L25

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res15.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L27 STRUCTURE UPLOADED

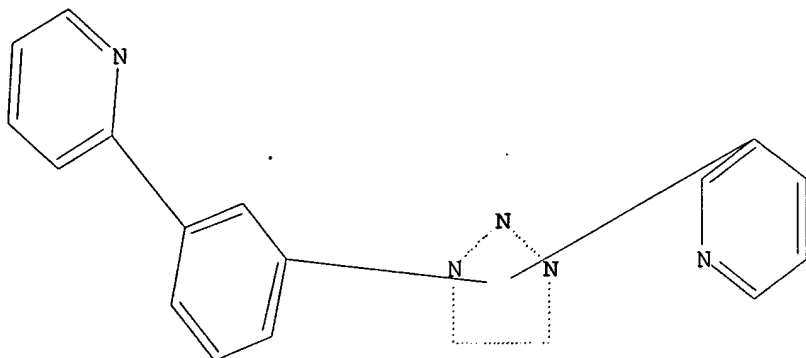
=> d

L27 HAS NO ANSWERS

L27 STR

Karen Cheng

10552362a



Structure attributes must be viewed using STN Express query preparation.

=> s 127 full

FULL SEARCH INITIATED 14:33:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

0 ANSWERS

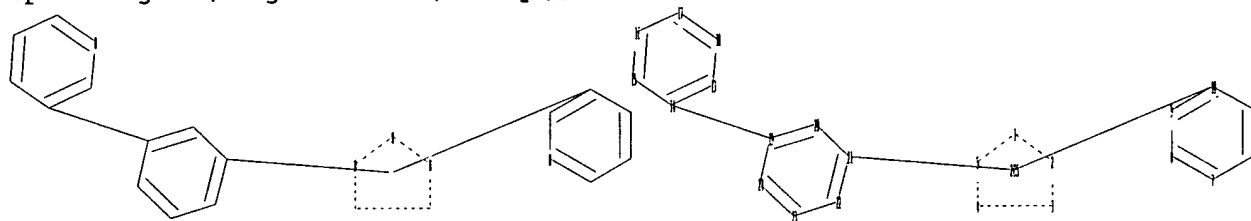
SEARCH TIME: 00.00.01

L28

0 SEA SSS FUL L27

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res16.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

14-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15

15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24

19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Karen Cheng

10552362a

Match level :

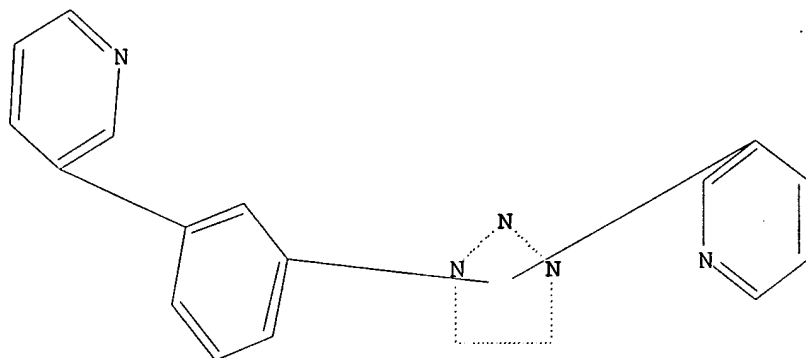
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L29 STRUCTURE UPLOADED

=> d

L29 HAS NO ANSWERS

L29 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l29 full

FULL SEARCH INITIATED 14:33:57 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

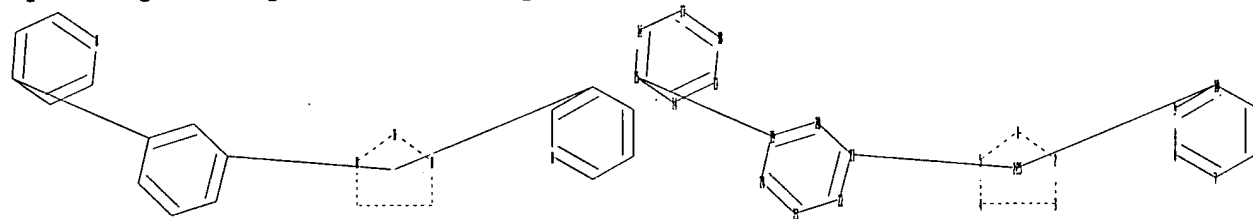
0 ANSWERS

SEARCH TIME: 00.00.01

L30 0 SEA SSS FUL L29

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res17.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

Karen Cheng

10552362a

15-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L31 STRUCTURE UPLOADED

=> s l31 full

FULL SEARCH INITIATED 14:34:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

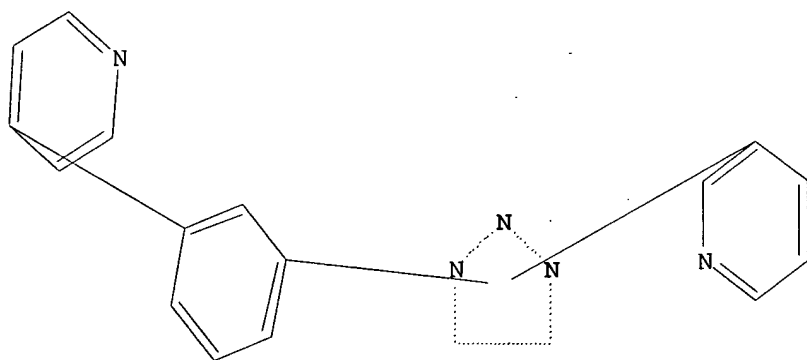
SEARCH TIME: 00.00.01

L32 0 SEA SSS FUL L31

=> d

L32 HAS NO ANSWERS

L31 STR



Structure attributes must be viewed using STN Express query preparation.

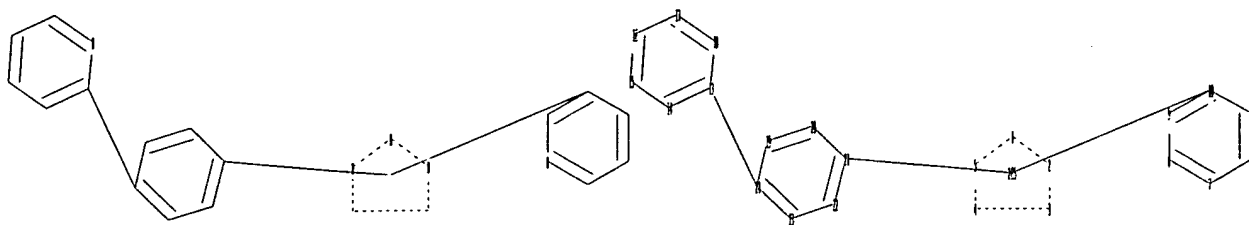
L32 0 SEA FILE=REGISTRY SSS FUL L31

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res18.str

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10552362a



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

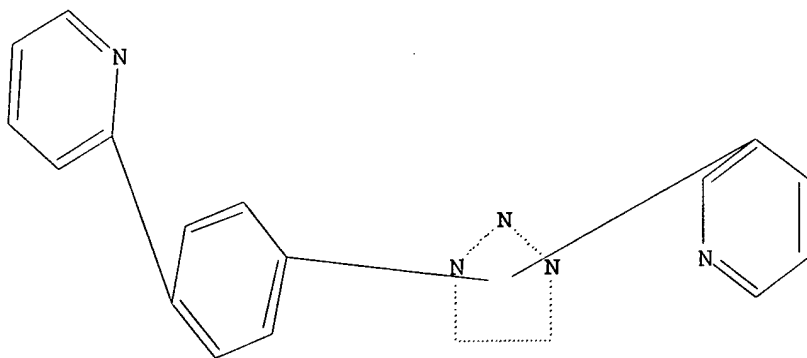
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L33 STRUCTURE UPLOADED

=> d

L33 HAS NO ANSWERS

L33 STR



Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l33 full

FULL SEARCH INITIATED 14:35:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

0 ANSWERS

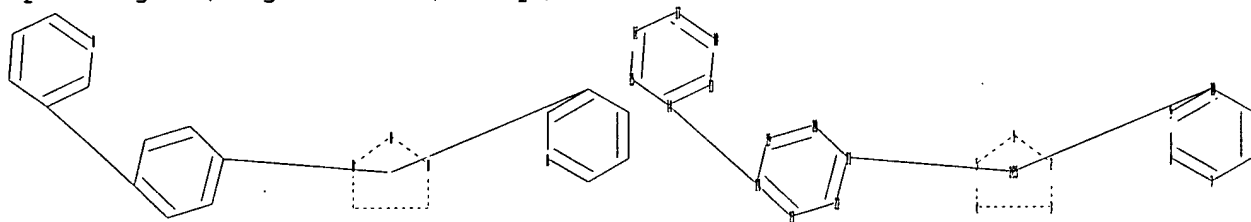
SEARCH TIME: 00.00.01

L34

0 SEA SSS FUL L33

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res19.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

14-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L35 STRUCTURE UPLOADED

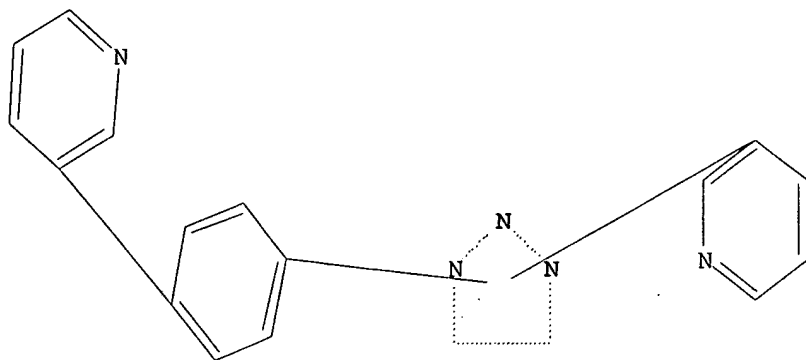
=> d

L35 HAS NO ANSWERS

L35 STR

Karen Cheng

10552362a



Structure attributes must be viewed using STN Express query preparation.

=> s l35 full

FULL SEARCH INITIATED 14:35:58 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

0 ANSWERS

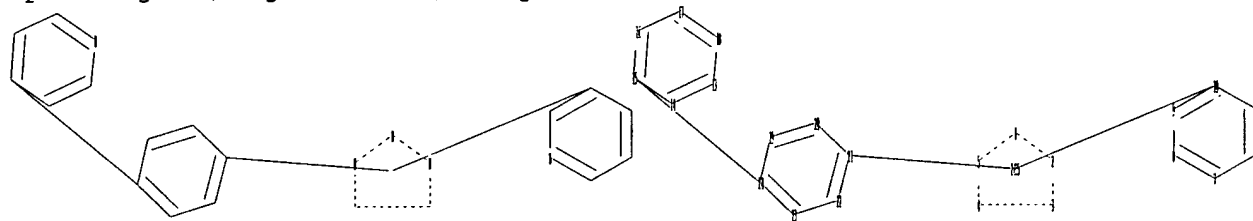
SEARCH TIME: 00.00.01

L36

0 SEA SSS FUL L35

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res20.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

15-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15

15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24

19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Karen Cheng

10552362a

Match level :

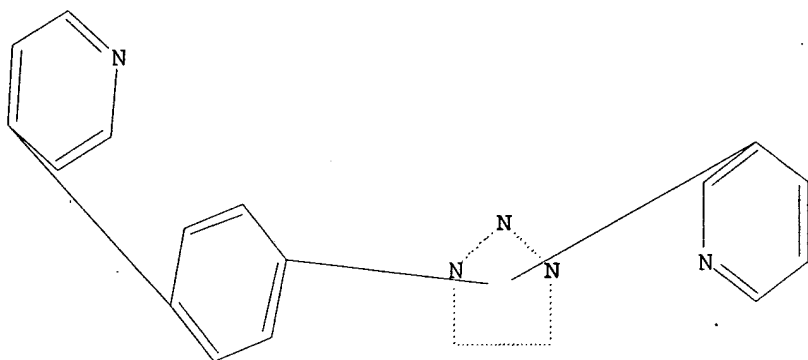
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L37 STRUCTURE UPLOADED

=> d

L37 HAS NO ANSWERS

L37 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l37 full

FULL SEARCH INITIATED 14:36:33 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

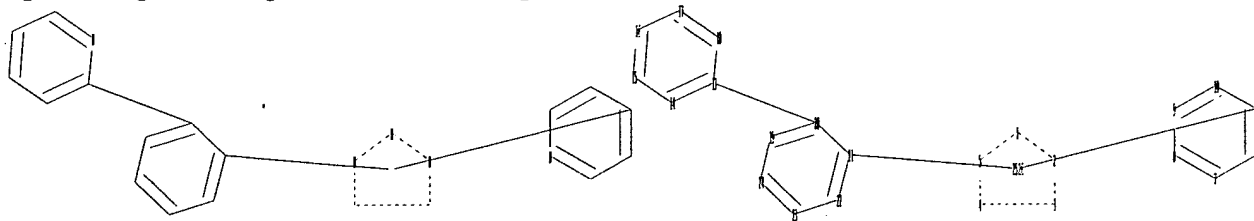
0 ANSWERS

SEARCH TIME: 00.00.01

L38 0 SEA SSS FUL L37

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res21.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

Karen Cheng

10552362a

13-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

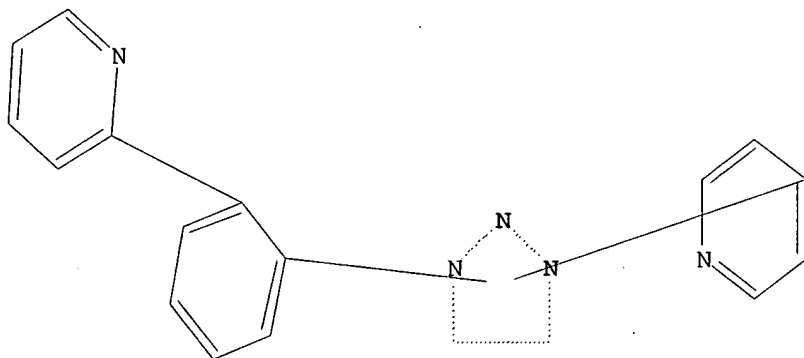
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L39 STRUCTURE UPLOADED

=> d

L39 HAS NO ANSWERS

L39 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l39 full

FULL SEARCH INITIATED 14:37:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

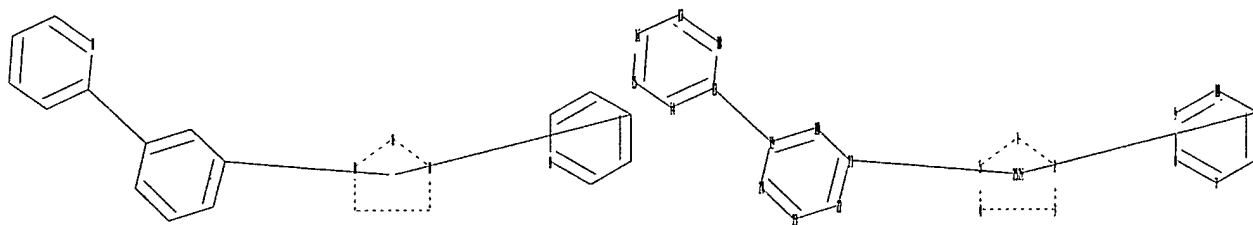
L40 0 SEA SSS FUL L39

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res22.str

Karen Cheng

10552362a



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

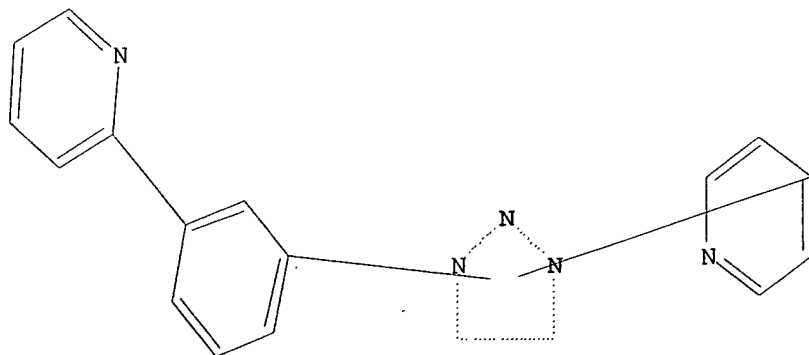
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L41 STRUCTURE UPLOADED

=> d

L41 HAS NO ANSWERS

L41 STR



Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l41 full

FULL SEARCH INITIATED 14:38:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

0 ANSWERS

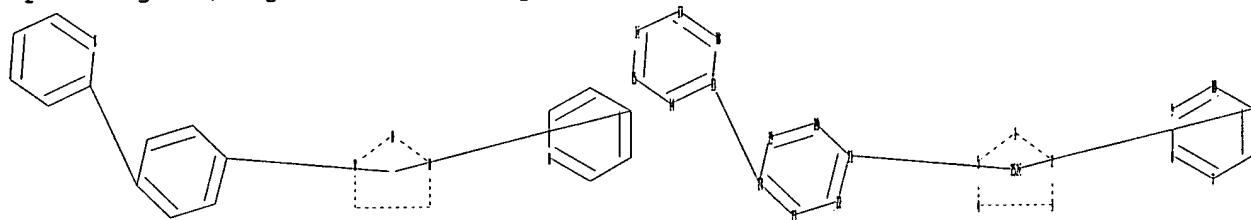
SEARCH TIME: 00.00.01

L42

0 SEA SSS FUL L41

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res23.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15

15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24

19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L43 STRUCTURE UPLOADED

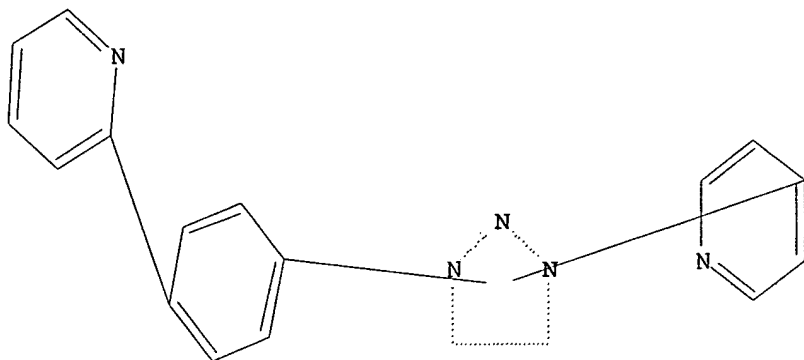
=> d

L43 HAS NO ANSWERS

L43 STR

Karen Cheng

10552362a



Structure attributes must be viewed using STN Express query preparation.

=> s l43 full

FULL SEARCH INITIATED 14:38:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

100.0% PROCESSED 1185 ITERATIONS

0 ANSWERS

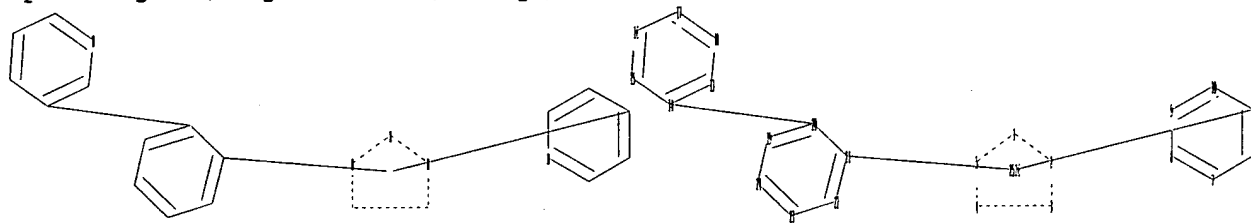
SEARCH TIME: 00.00.01

L44

0 SEA SSS FUL L43

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res24.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

14-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-20

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

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10552362a

Match level :

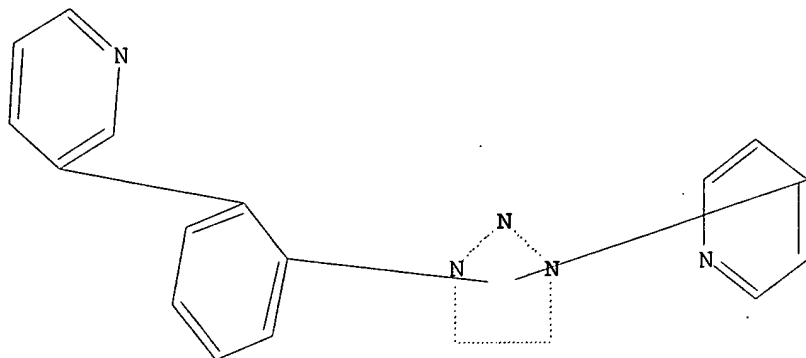
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21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L45 STRUCTURE UPLOADED

=> d

L45 HAS NO ANSWERS

L45 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l45 full

FULL SEARCH INITIATED 14:39:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

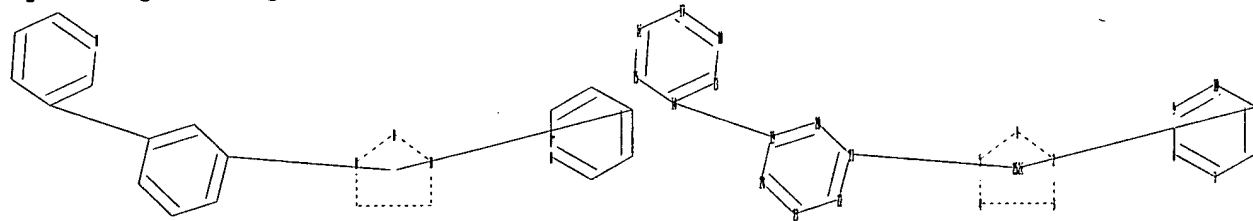
0 ANSWERS

SEARCH TIME: 00.00.01

L46 0 SEA SSS FUL L45

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res25.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

Karen Cheng

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14-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

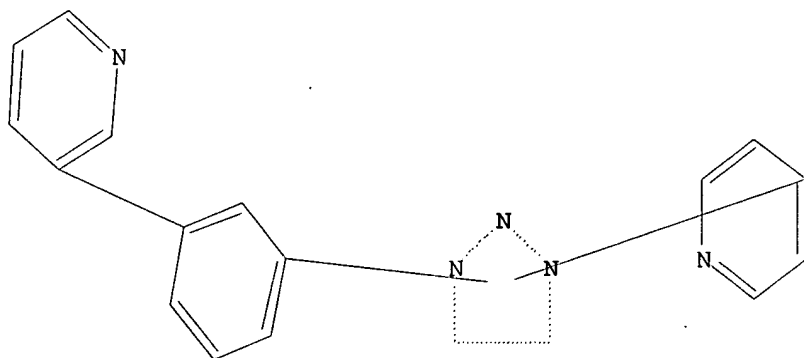
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L47 STRUCTURE UPLOADED

=> d

L47 HAS NO ANSWERS

L47 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l47 full

FULL SEARCH INITIATED 14:40:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

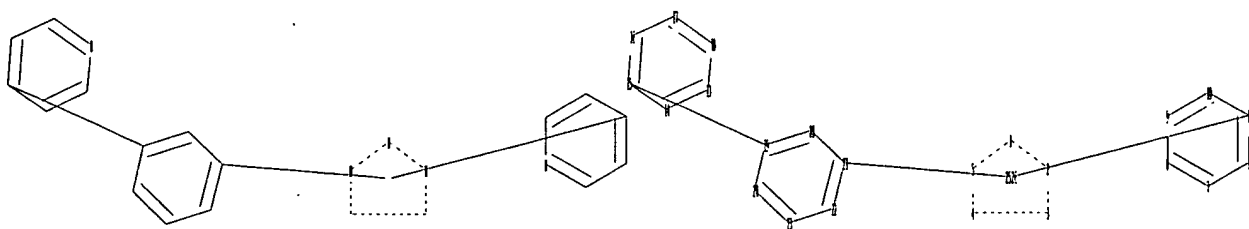
L48 0 SEA SSS FUL L47

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res26.str

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ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

15-19

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-19

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

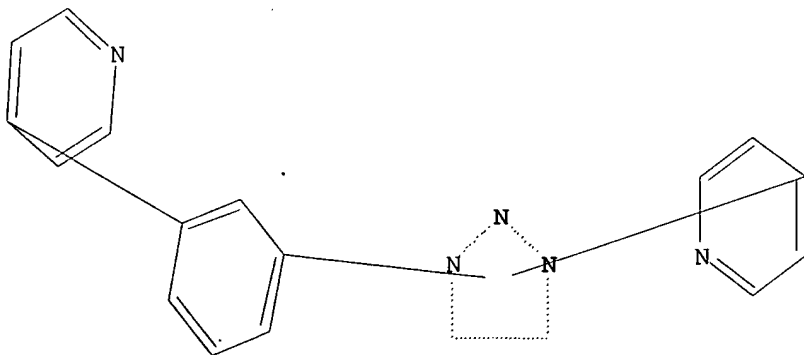
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L49 STRUCTURE UPLOADED

=> d

L49 HAS NO ANSWERS

L49 STR



Karen Cheng

10552362a

Structure attributes must be viewed using STN Express query preparation.

=> s l49 full

FULL SEARCH INITIATED 14:40:46 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

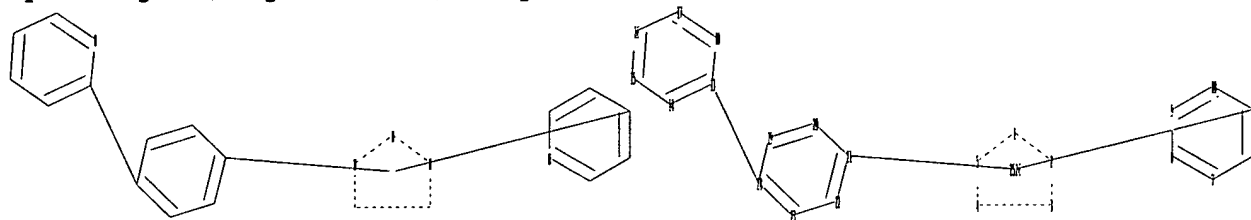
SEARCH TIME: 00.00.01

L50

0 SEA SSS FUL L49

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res27.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

13-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15

15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

13-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24

19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L51 STRUCTURE UPLOADED

=> s l51 full

FULL SEARCH INITIATED 14:41:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1185 TO ITERATE

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100.0% PROCESSED 1185 ITERATIONS
SEARCH TIME: 00.00.01

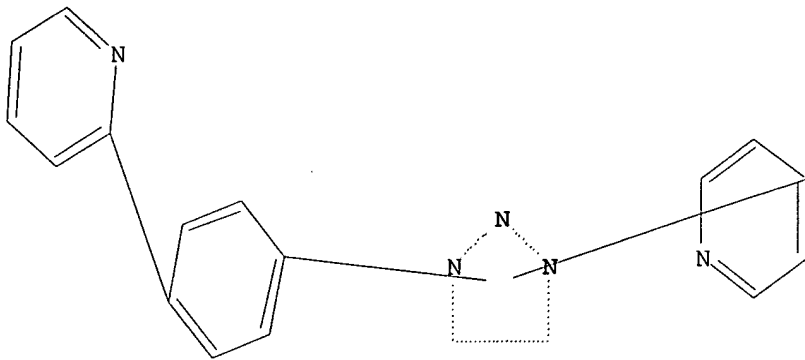
0 ANSWERS

L52 0 SEA SSS FUL L51

=> d l51

L51 HAS NO ANSWERS

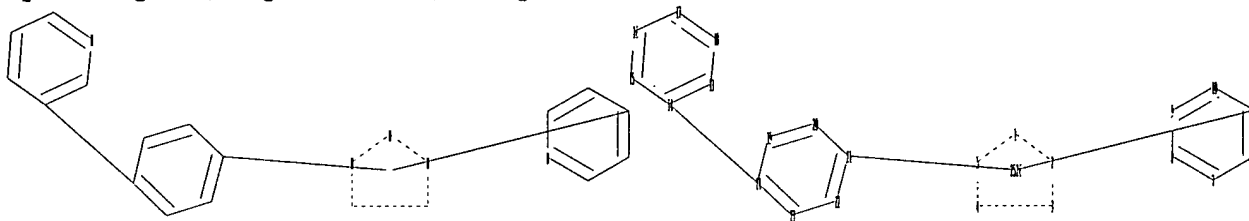
L51 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res28.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

14-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

14-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

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10552362a

Match level :

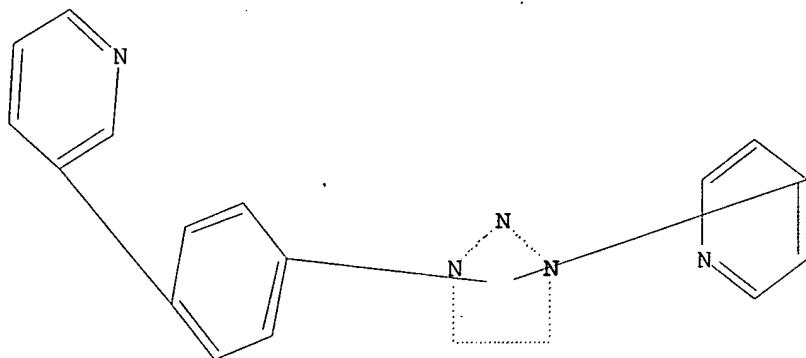
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12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L53 STRUCTURE UPLOADED

=> d

L53 HAS NO ANSWERS

L53 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l53 full

FULL SEARCH INITIATED 14:42:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 614 TO ITERATE

100.0% PROCESSED 614 ITERATIONS

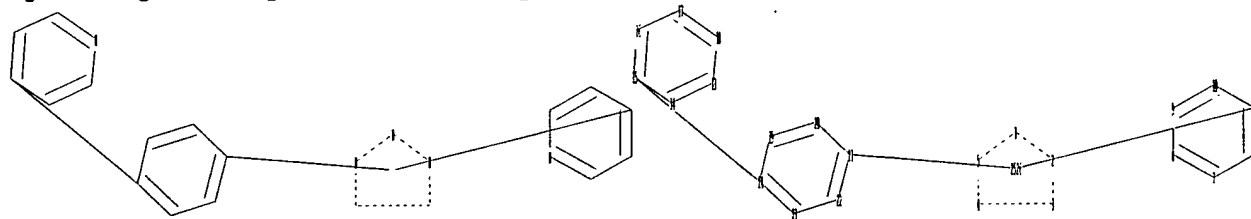
0 ANSWERS

SEARCH TIME: 00.00.01

L54 0 SEA SSS FUL L53

=>

Uploading C:\Program Files\Stnexp\Queries\10552362res29.str



ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

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15-24

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15
15-16 16-17 17-18 19-24 19-20 20-21 21-22 22-23 23-24

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds :

15-24

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-18 13-14 14-15 15-16 16-17 17-18 19-24
19-20 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 7 : 13 : 19 :

Match level :

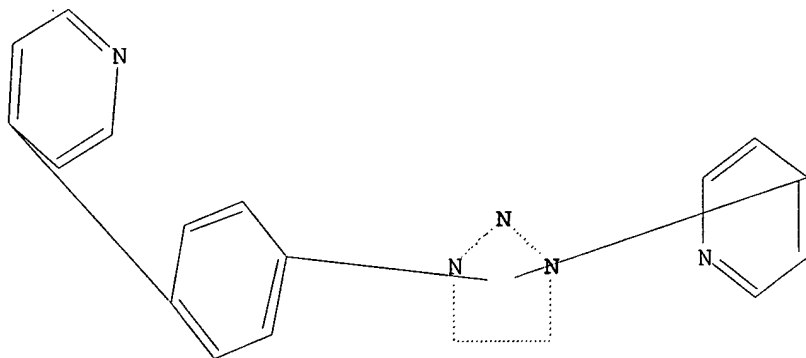
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L55 STRUCTURE UPLOADED

=> d

L55 HAS NO ANSWERS

L55 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l55 full

FULL SEARCH INITIATED 14:42:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 435 TO ITERATE

100.0% PROCESSED 435 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L56 0 SEA SSS FUL L55

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

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FULL ESTIMATED COST

4651.20 4651.41

FILE 'CAPLUS' ENTERED AT 14:42:52 ON 02 APR 2007
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FILE LAST UPDATED: 1 Apr 2007 (20070401/ED)

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=> d his

(FILE 'HOME' ENTERED AT 14:20:17 ON 02 APR 2007)

FILE 'REGISTRY' ENTERED AT 14:20:27 ON 02 APR 2007

L1	STRUCTURE UPLOADED
L2	0 S L1 FULL
L3	STRUCTURE UPLOADED
L4	2 S L3 FULL
L5	STRUCTURE UPLOADED
L6	STRUCTURE UPLOADED
L7	8 S L6 FULL
L8	STRUCTURE UPLOADED
L9	0 S L8 FULL
L10	STRUCTURE UPLOADED
L11	2 S L10 FULL
L12	STRUCTURE UPLOADED
L13	0 S L12 FULL
L14	STRUCTURE UPLOADED
L15	0 S L14 FULL
L16	STRUCTURE UPLOADED
L17	STRUCTURE UPLOADED
L18	0 S L17 FULL
L19	STRUCTURE UPLOADED
L20	0 S L19 FULL
L21	STRUCTURE UPLOADED
L22	0 S L21 FULL
L23	STRUCTURE UPLOADED
L24	0 S L23 FULL
L25	STRUCTURE UPLOADED
L26	0 S L25 FULL
L27	STRUCTURE UPLOADED
L28	0 S L27 FULL
L29	STRUCTURE UPLOADED

Karen Cheng

10552362a

L30	0 S L29 FULL
L31	STRUCTURE UPLOADED
L32	0 S L31 FULL
L33	STRUCTURE UPLOADED
L34	0 S L33 FULL
L35	STRUCTURE UPLOADED
L36	0 S L35 FULL
L37	STRUCTURE UPLOADED
L38	0 S L37 FULL
L39	STRUCTURE UPLOADED
L40	0 S L39 FULL
L41	STRUCTURE UPLOADED
L42	0 S L41 FULL
L43	STRUCTURE UPLOADED
L44	0 S L43 FULL
L45	STRUCTURE UPLOADED
L46	0 S L45 FULL
L47	STRUCTURE UPLOADED
L48	0 S L47 FULL
L49	STRUCTURE UPLOADED
L50	0 S L49 FULL
L51	STRUCTURE UPLOADED
L52	0 S L51 FULL
L53	STRUCTURE UPLOADED
L54	0 S L53 FULL
L55	STRUCTURE UPLOADED
L56	0 S L55 FULL

FILE 'CAPLUS' ENTERED AT 14:42:52 ON 02 APR 2007

```
=> s (l4 or l7 or l11)
      1 L4
      1 L7
      1 L11
L57      1 (L4 OR L7 OR L11)
```

```
=> d ibib abs hitstr tot
```

10552362a

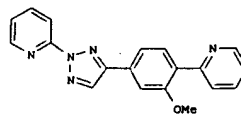
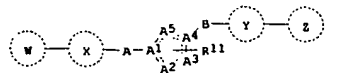
L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:878275 CAPLUS
 DOCUMENT NUMBER: 141:366235
 TITLE: Preparation of diaryl substituted triazole modulators of metabotropic glutamate receptor-5
 INVENTOR(S): Cosford, Nicholas D. P.; Roppe, Jeffrey R.; Tehrani, Lida R.; Wang, Bowei
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 42 pp.
 DOCUMENT TYPE: CODEN: PIXXD2
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: English
 PATENT INFORMATION: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089306	A2	20041021	WO 2004-US9750	20040331
WO 2004089306	A3	20050217		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004227833	A1	20041021	AU 2004-227833	20040331
CA 2521396	A1	20041021	CA 2004-2521396	20040331
EP 1613617	A2	20060111	EP 2004-758603	20040331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1795186	A	20060628	CN 2004-80014560	20040331
JP 2006522131	T	20060928	JP 2006-509488	20040331
US 2003-462796P P 20030404				
PRIORITY APPLN. INFO.: WO 2004-US9750 W 20040331				

OTHER SOURCE(S): MARPAT 141:366235
 GI

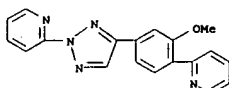
L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. represented by the formula I [wherein X, Y = independently (hetero)aryl, and at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B; A1-A5 = independently N or C, three of them are N, and one of A1 and A4 must be N, but not both A1 and A4 are H; A, B = independently (hetero)alkyl, alkylsulfonylalkyl, alkylcarbonylalkyl, etc.; W, Z = independently (un)substituted (hetero)cycloalkyl, alkyl(hetero)aryl; R11 = halo, alkyl, alkoxy, etc.; and pharmaceutically acceptable salts thereof] were prepared as modulators of metabotropic glutamate receptor-5 (mGluR5). For example, reaction of 2-[2-methoxy-4-(1H-1,2,3-triazol-4-yl)phenyl]pyridine with 1-fluoropyridinium triflate gave II. The prepared I were tested for mGluR5 inhibitory activity with IC50 value of less than 10 μ M in the calcium flux assay or inhibition of >50 % at a concentration of 100 μ M in the PI assay. Thus, I and their pharmaceutical compns. are useful as modulators of mGluR5 for the treatment of panic, and bipolar disorder, as well as in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, obesity, drug addiction, drug abuse, drug withdrawal and other diseases (no data).

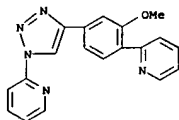
IT 777864-97-8P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of diaryl substituted triazole modulators of metabotropic glutamate receptor-5)
 RN 777864-97-8 CAPLUS
 CN Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



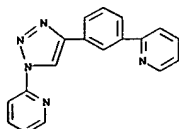
● HCl

IT 777864-98-9P 777864-99-0P 777865-00-6P
 777865-01-7P 777865-02-8P 777865-03-9P
 777865-04-0P 777865-05-1P 777865-06-2P
 777865-08-4P 777865-09-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of diaryl substituted triazole modulators of metabotropic glutamate receptor-5)
 RN 777864-98-9 CAPLUS
 CN Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

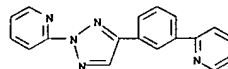
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 CN Pyridine, 2-[4-[3-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]- (9CI) (CA INDEX NAME)



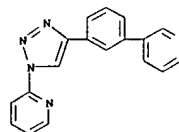
Karen Cheng

L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

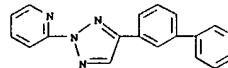
RN 777865-00-6 CAPLUS
 CN Pyridine, 2-[4-[3-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]- (9CI) (CA INDEX NAME)



RN 777865-01-7 CAPLUS
 CN Pyridine, 2-[4-[3-(3-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]- (9CI) (CA INDEX NAME)



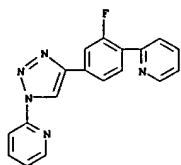
RN 777865-02-8 CAPLUS
 CN Pyridine, 2-[4-[3-(3-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]- (9CI) (CA INDEX NAME)



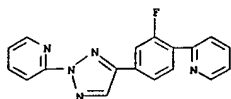
RN 777865-03-9 CAPLUS
 CN Pyridine, 2-[4-[3-fluoro-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]- (9CI) (CA INDEX NAME)

10552362a

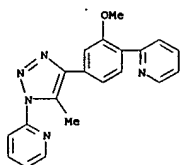
L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 777865-04-0 CAPLUS
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(9CI) (CA INDEX NAME)

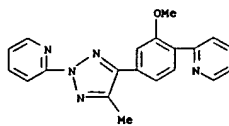


RN 777865-05-1 CAPLUS
CN Pyridine, 2-[2-methoxy-4-[5-methyl-1-(2-pyridinyl)-1H-1,2,3-triazol-4-yl]phenyl]-
(9CI) (CA INDEX NAME)

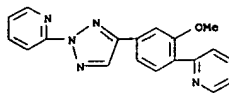


RN 777865-06-2 CAPLUS
CN Pyridine, 2-[2-methoxy-4-[5-methyl-2-(2-pyridinyl)-2H-1,2,3-triazol-4-yl]phenyl]-
(9CI) (CA INDEX NAME)

L57 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 777865-08-4 CAPLUS
CN Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-2H-1,2,3-triazol-2-yl]-
(9CI) (CA INDEX NAME)



RN 777865-09-5 CAPLUS
CN Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-1,2,3-triazol-1-yl]-
(9CI) (CA INDEX NAME)

